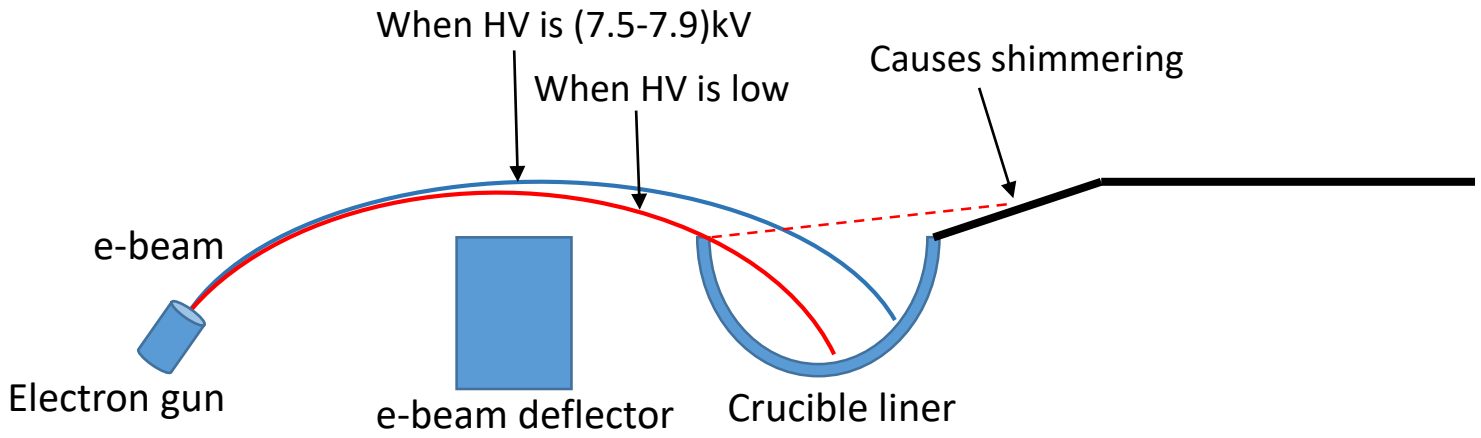
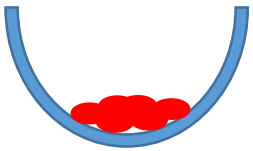
EvoVac: Using e-beam apparatus





Not the best way to place the source material in the crucible liner.

Placing the source material this allows for maximum exposure of the material to e-beam.

Single-ion anisotropy in rare-earth metals (*4f* Lanthanides)

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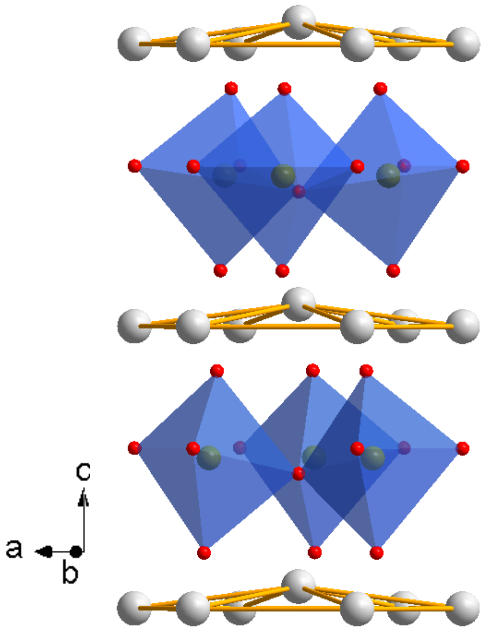
4f- Rare-earths ions (R^{3+}): Lanthanides



Hexagonal $RFeO_3$

Valence: $4f^1$- $4f^{14}$

Highly anisotropic electron distribution

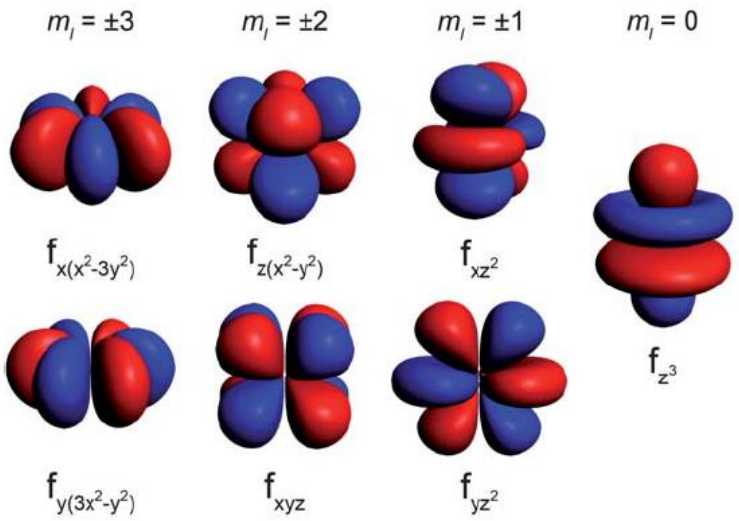
← *4f* rare-earths in *3+* oxidation state.

IUPAC Periodic Table of the Elements

1	2											13	14	15	16	17	18
																	2 He helium 4.003
	4 Be beryllium 9.012											5 B boron [10.80, 10.83]	6 C carbon [12.00, 12.02]	7 N nitrogen [14.00, 14.01]	8 O oxygen [15.99, 16.00]	9 F fluorine 19.00	10 Ne neon 20.18
11 Na sodium 22.99	12 Mg magnesium [24.30, 24.31]	3	4	5	6	7	8	9	10	11	12	13 Al aluminium 26.98	14 Si silicon [28.08, 28.09]	15 P phosphorus 30.97	16 S sulfur [32.05, 32.08]	17 Cl chlorine [35.44, 35.46]	18 Ar argon 39.95
19 K potassium 39.10	20 Ca calcium 40.08	21 Sc scandium 44.96	22 Ti titanium 47.87	23 V vanadium 50.94	24 Cr chromium 52.00	25 Mn manganese 54.94	26 Fe iron 55.85	27 Co cobalt 58.93	28 Ni nickel 58.69	29 Cu copper 63.55	30 Zn zinc 65.38(2)	31 Ga gallium 69.72	32 Ge germanium 72.63	33 As arsenic 74.92	34 Se selenium 78.96(3)	35 Br bromine [79.90, 79.91]	36 Kr krypton 83.80
37 Rb rubidium 85.47	38 Sr strontium 87.62	39 Y yttrium 88.91	40 Zr zirconium 91.22	41 Nb niobium 92.91	42 Mo molybdenum 95.96(2)	43 Tc technetium	44 Ru ruthenium 101.1	45 Rh rhodium 102.9	46 Pd palladium 106.4	47 Ag silver 107.9	48 Cd cadmium 112.4	49 In indium 114.8	50 Sn tin 118.7	51 Sb antimony 121.8	52 Te tellurium 127.6	53 I iodine 126.9	54 Xe xenon 131.3
55 Cs caesium 132.9	56 Ba barium 137.3	57-71 lanthanoids	72 Hf hafnium 178.5	73 Ta tantalum 180.9	74 W tungsten 183.8	75 Re rhenium 186.2	76 Os osmium 190.2	77 Ir iridium 192.2	78 Pt platinum 195.1	79 Au gold 197.0	80 Hg mercury 200.6	81 Tl thallium [204.3, 204.4]	82 Pb lead 207.2	83 Bi bismuth 209.0	84 Po polonium	85 At astatine	86 Rn radon
87 Fr francium	88 Ra radium	89-103 actinoids	104 Rf rutherfordium	105 Db dubnium	106 Sg seaborgium	107 Bh bohrium	108 Hs hassium	109 Mt meitnerium	110 Ds darmstadtium	111 Rg roentgenium	112 Cn copernicium		114 Fl flerovium		116 Lv livermorium		

57 La lanthanum 138.9	58 Ce cerium 140.1	59 Pr praseodymium 140.9	60 Nd neodymium 144.2	61 Pm promethium	62 Sm samarium 150.4	63 Eu europium 152.0	64 Gd gadolinium 157.3	65 Tb terbium 158.9	66 Dy dysprosium 162.5	67 Ho holmium 164.9	68 Er erbium 167.3	69 Tm thulium 168.9	70 Yb ytterbium 173.1	71 Lu lutetium 175.0
89 Ac actinium	90 Th thorium 232.0	91 Pa protactinium 231.0	92 U uranium 238.0	93 Np neptunium	94 Pu plutonium	95 Am americium	96 Cm curium	97 Bk berkelium	98 Cf californium	99 Es einsteinium	100 Fm fermium	101 Md mendelevium	102 No nobelium	103 Lr lawrencium

Electron distribution in *4f* lanthanides



Representations of the 4f orbitals

Highest magnitude m_j- most oblate shape
Lowest magnitude m_j - most prolate shape

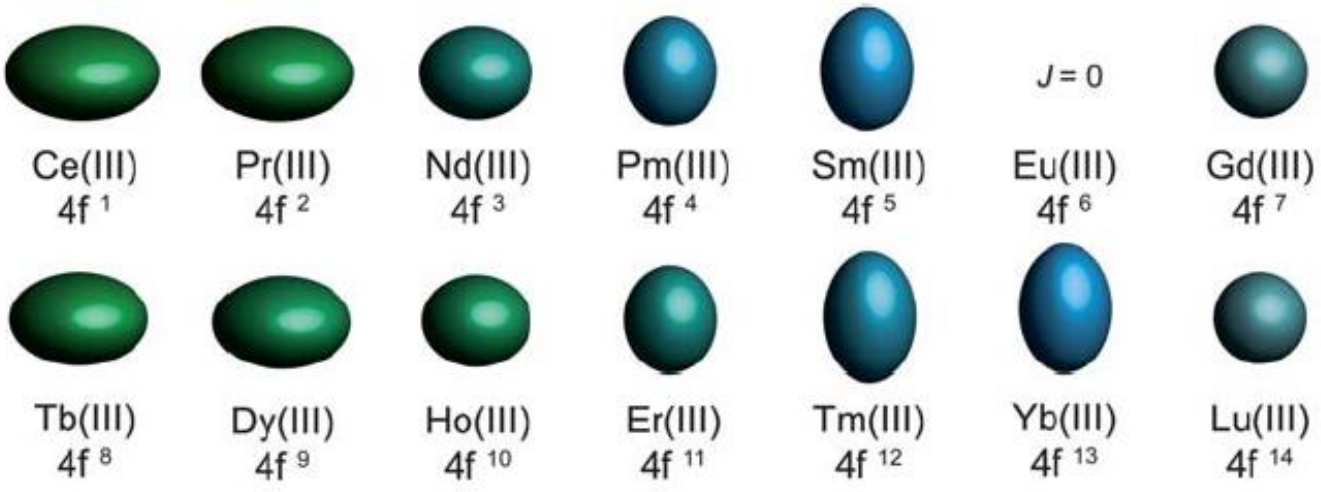
High m_j → high net magnetic moment along *z*-axis

Rare-earths metals exhibit strong spin-orbit (LS) coupling as opposed to their 3d transition metal counterparts.

Consequently, the "good" quantum number is ***j*** (total angular momentum)and not ***s***.

This leads to weaker coupling between electronic distribution in rare-earth ions and the crystal field due to ligands.
→ Crystal field is treated as a perturbation on LS coupling term in the Hamiltonian. (This is in stark contrast with the way transition metal ions behave.)

Electron distribution in *4f* lanthanides



Quadrupole approximations of the *4f*-shell electron distribution for the tripositive lanthanides.

Values are calculated using the total angular momentum quantum number (*J*), the Stevens coefficient of second order (α) and the radius of the *4f* shell squared $\langle r^2 \rangle$.

Europium is not depicted is a *J = 0* ground state.

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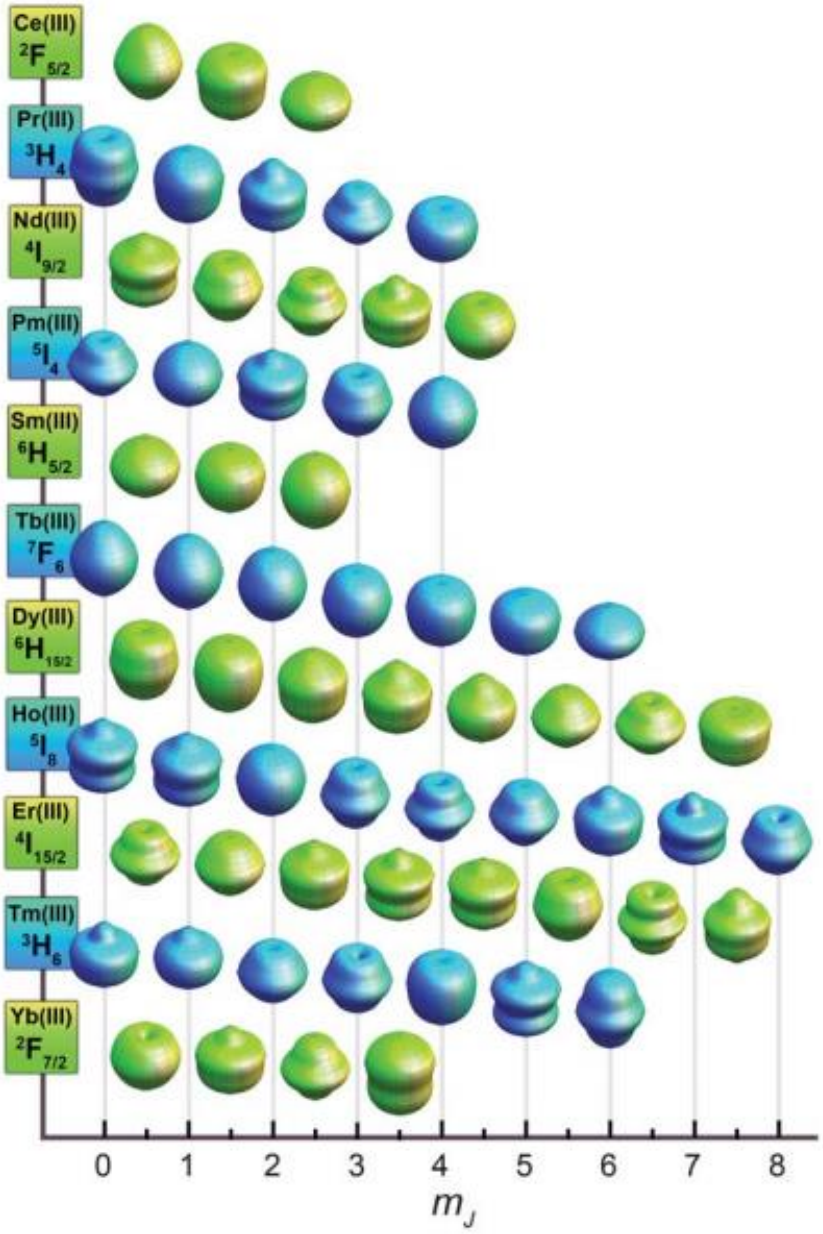
4f Electron distribution vs. m_j

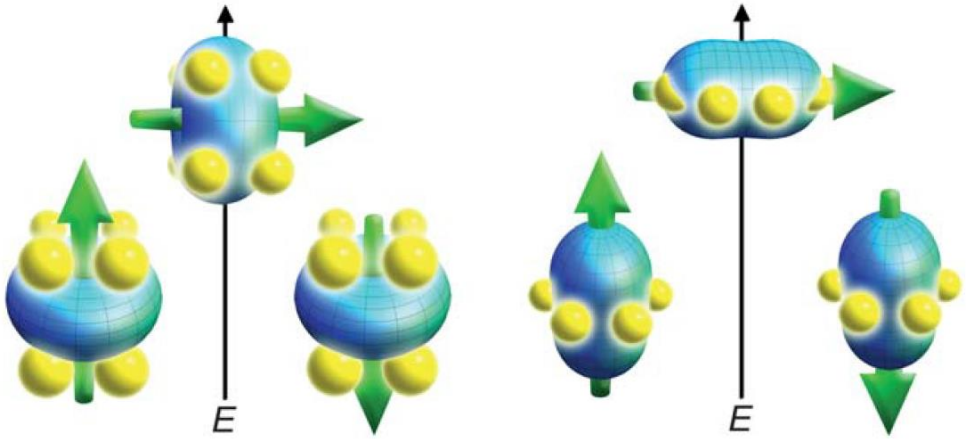


In the absence of crystal field, all m_j states are degenerate.

Applications in magnetic materials would require crystal fields that minimize the energy of highest m_j states.

This would lead to doubly-degenerate ground state with high m_j states.
→ Augment anisotropy.

Low and High energy configurations



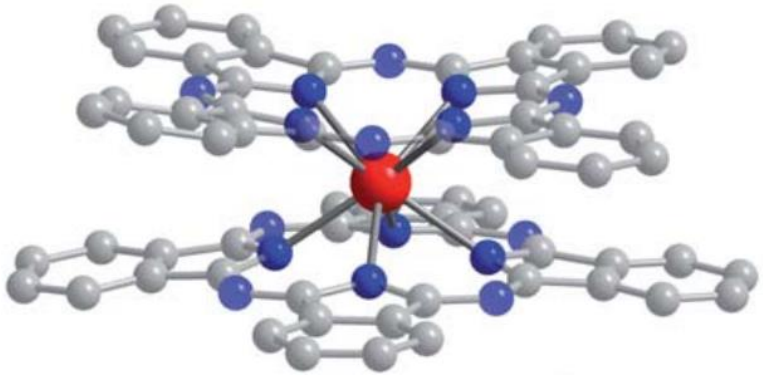
4f ion with oblate electron density

4f ion with prolate electron density

Depictions of low- and high-energy configurations of the f-orbital electron density with respect to the crystal field environment for an oblate and a prolate electron density.

- The green arrow represents the orientation of the spin angular momentum coupled to the orbital moment.
- For the **oblate electron density**, an **axial** ‘‘sandwich’’- type crystal field minimizes the energy of the $m_J = J$ (high moment) state.
- For the **prolate electron density**, an **equatorial** ‘‘sandwich’’- type crystal field minimizes the energy of the $m_J = J$ (high moment) state.

Materials using strong single-ion anisotropy

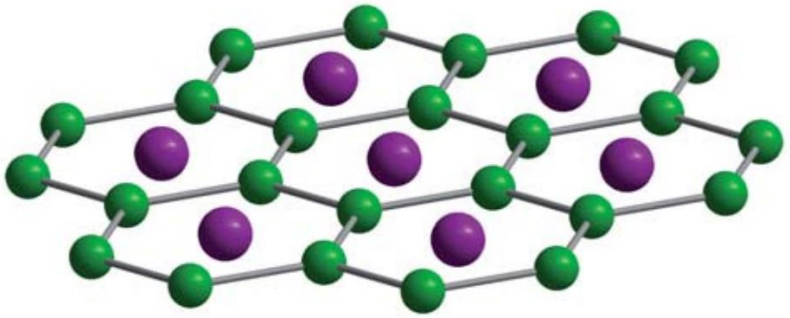


$[TbPc_2]^-$

- **Pc_2^-** = phthalocyanine

Red-Terbium; blue-nitrogen; gray-carbon

- **Tb** here is **an oblate ion**.
- Axial ligands reduce the energy of the highest m_j.
- Hence, stabilizing the maximum moment state.
- The structure has high and stable out-of-plane magnetic moment.



$SmCo_5$

- **Sm** here is **a prolate ion**.
- Equatorial ligands reduce the energy of the highest m_j.
- Hence, stabilizing the maximum moment state.
- The structure has high and stable out-of-plane magnetic moment.

Thank you!